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Title: Optimizing and Extending the Functionality of EXARL for Scalable

Reinforcement Learning

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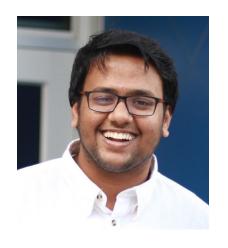


Optimizing and Extending the Functionality of EXARL for Scalable Reinforcement Learning

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August 5, 2021

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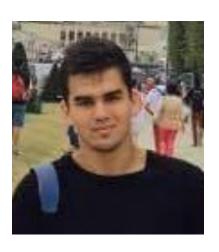
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Introduction to **Reinforcement Learning**

- A subset of machine learning wherein an agent interacts and learns from its environment over time.
- The agent receives a **state** from its environment and selects an action according to its **policy** (a mapping from states to actions).
- The agent then receives the **next** state and a scalar reward from the environment.
- Goal is to achieve the maximum amount of reward over time.

Environment

Agent

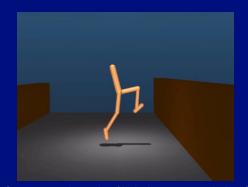
Action

Policy

State

Reward

Next State





Introduction to EXARL

Easily eXtendable Architecture for Reinforcement Learning



- EXARL is a scalable reinforcement learning framework for scientific environments.
 - Originally developed as part of ExaLearn through Exascale Computing Project (ECP)
- Why scalable?
 - Scientific environments are *complex* and often take a long time to run, even while running in parallel
 - Ability to run on multiple nodes reduces this time
- The **goal of EXARL** is to make prototyping and reproducing scientific RL studies easier by...
 - Providing a framework of agents, environments, workflows that are easy to add and implement
 - Having a user-friendly front-end interface (written in python)
 - Supporting different hardware and software infrastructures



EXARL architecture

Agent is decomposed into **Actor** and Learner

Actor:

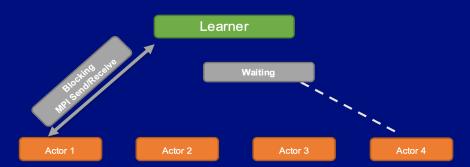
- Gets the model/policy from the learner
- Interacts with the environment by taking action based on the model/policy
- Receives the trajectories (state, action, next-state, reward) from the environment
- Sends the batched trajectories to the learner to update the policy

Learner:

- Receives trajectories from actor
- Updates the model/policy based on the new data
- Sends the updated policy to the actor
- **EXARL** provides a scalable framework for reinforcement learning
 - **Multiple actors & environments** to accelerate learning process
 - **Multiple learners** to accelerate policy update process

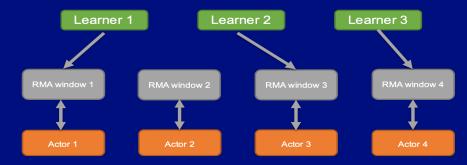


EXARL Implementation: Asynchronous vs RMA workflow



Asynchronous workflow:

- Blocking two-sided (MPI-Send/Recv) communication b/w actors and learners
- **Pros:** Actors receive recently updated policies
- **Cons:** Only has single-learner implementation, poor scalability, low policy update frequency



RMA asynchronous workflow:

- One-sided(MPI-RMA) communication b/w actors and learners
- **Pros:** Supports multiple learners, high policy update frequency – decoupled actors and learners
- Cons: Policy and experience lag between actors and learners



Overview

Main goal of the Co-Design Summer School 2021 is to provide algorithmic **improvements to EXARL framework**. This is in the form of:

Improving Performance

- Scaling asynchronous workflow to multiple learners
- Improve scalability/execution time of multi-learner workflows
- Accelerate Deep Q-Network (DQN) data generation pipeline

Adding Functionalities

- New agents: Advantage Actor Critic (A2C/A3C), Twin Delayed Deep Deterministic Policy Gradient (TD3)
- V-trace algorithm
- Priority Experience Replay





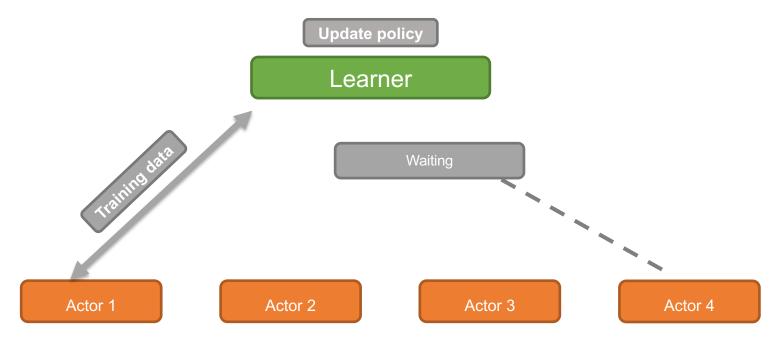






Building Multi-learner Asynchronous Workflow

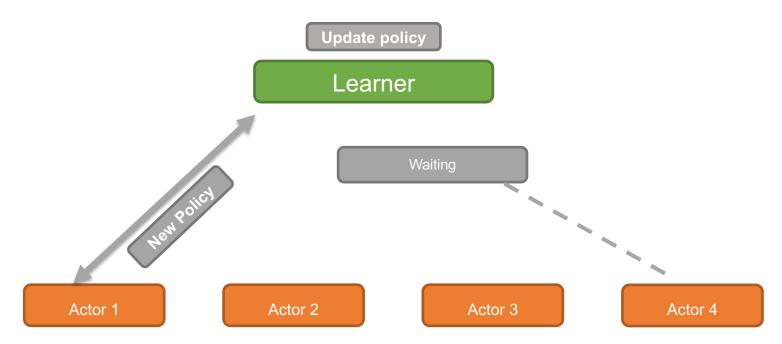
Current approach: Asynchronous workflow only supports single-learner





Building Multi-learner Asynchronous Workflow

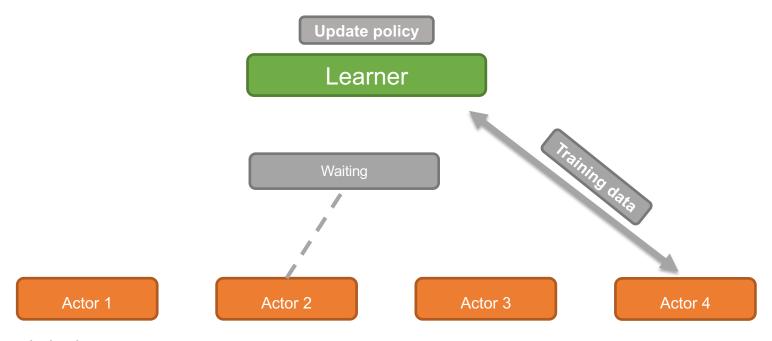
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Building Multi-learner Asynchronous Workflow

Current approach: Asynchronous workflow only supports single-learner

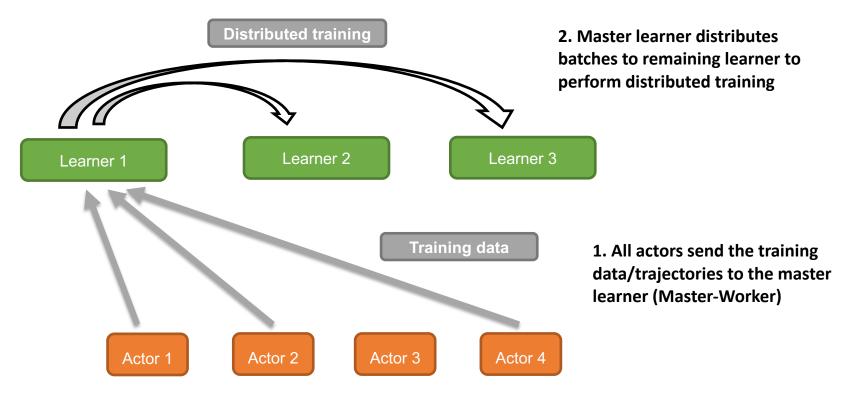


- Limitation:
 - Slow training time in case of multiple actors and/or fast environments



Multi-learner Asynchronous Workflow

• **Update**: Implemented multi-learner asynchronous workflow



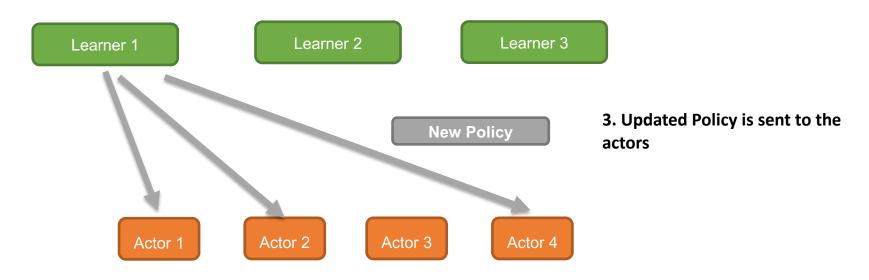


Multi-learner Asynchronous Workflow

• **Update**: Implemented multi-learner asynchronous workflow

Pros: Faster training

Cons: Low policy update frequency





Multi-learner Asynchronous Workflow: Results

Experimental Setup:

System: Darwin | Node: Intel Broadwell (36 cores)

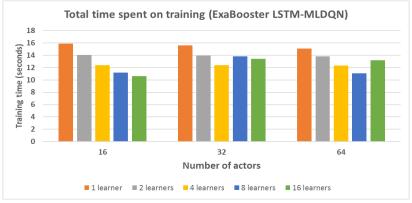
Partition: Scaling

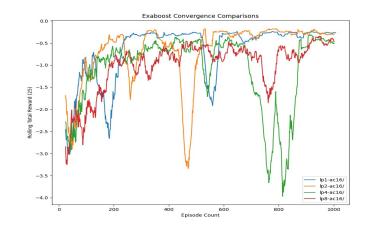
• Environment: ExaBooster

Episode count: 1000 | Step count: 200

Observations:

- Reduced training time with multiple learners
- Poor convergence with multiple learners
 - Low policy update frequency
- Multiple learner workflow more suitable for onpolicy agents
 - Policy update after every episode

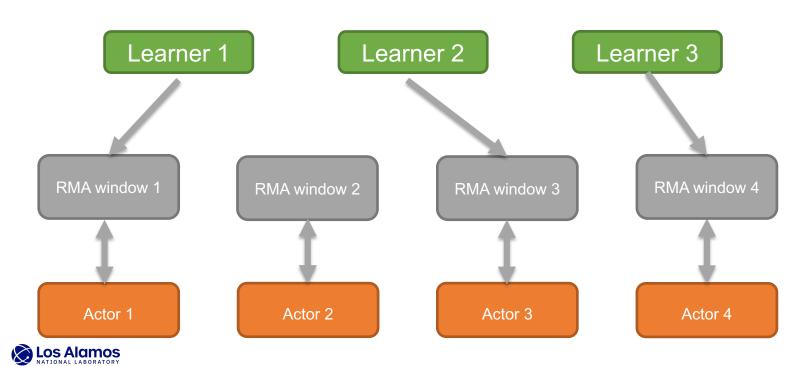




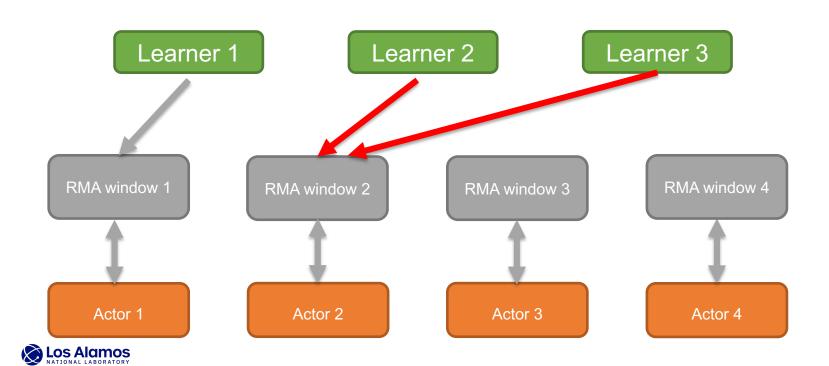


In Multi-learner RMA workflow, learner gets the training data from the actor's RMA window

Current approach: Each learner randomly selects one of the actor's RMA window



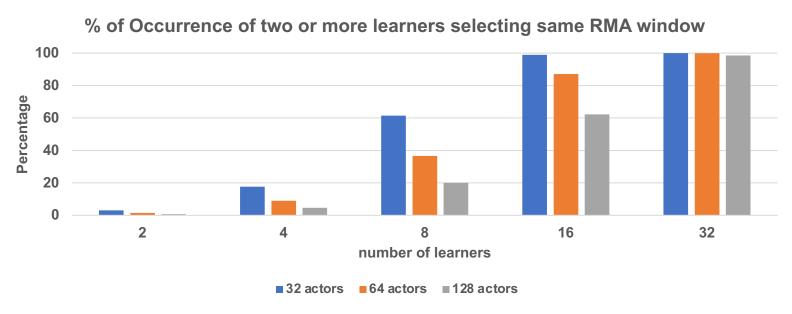
In Multi-learner RMA workflow, learner gets the training data from the actor's RMA window **Limitation:** Multiple learners access same actor window



Performed simulations to observe the frequency of such behaviour

Observations:

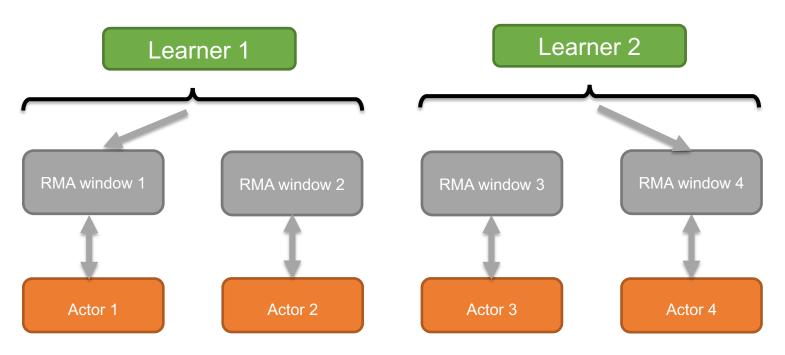
Significant occurrence when # of learners are at least 25% of the total actors





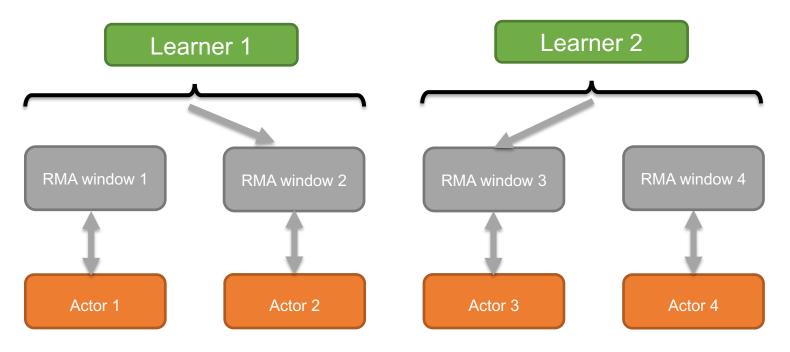
Proposed approach:

Allocate a set of actor RMA windows to each learner





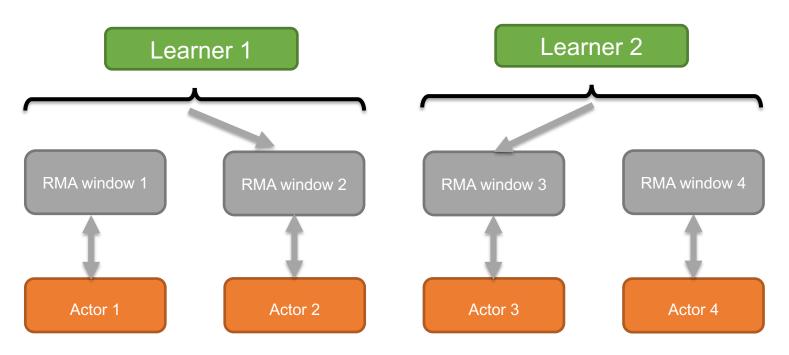
- Proposed approach:
 - Allocate a set of actor RMA windows to each learner





Advantages:

Guarantees no learner reads from the same actor's RMA window





Multi-learner RMA Window Selection Policy: Results

Experimental Setup:

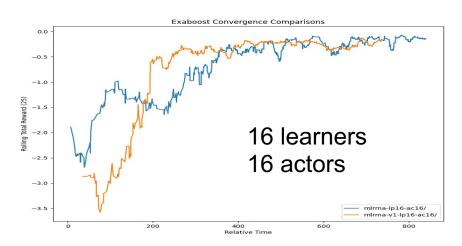
Environment: ExaBooster

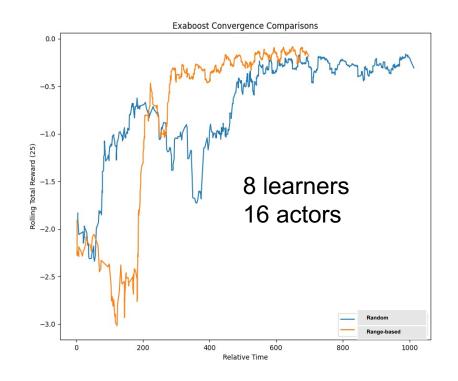
Episode count: 1000 Step count: 200

Action type: variable

Observations:

- Faster convergence
- Improvement in convergence is due to non redundant training data during distributed learning







Multi-learner RMA Window Selection Policy: Results

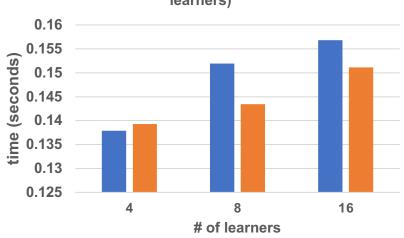
Experimental Setup:

Environment: ExaBooster

Episode count: 1000 Step count: 200

Action type: fixed

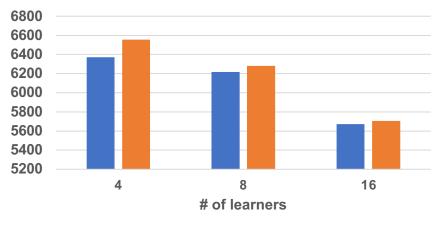
RMA Window Get time (averaged across all learners)



Observations:

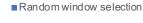
- Faster convergence
- (Not significant) reduction in access time.

Number of RMA Window Accesses



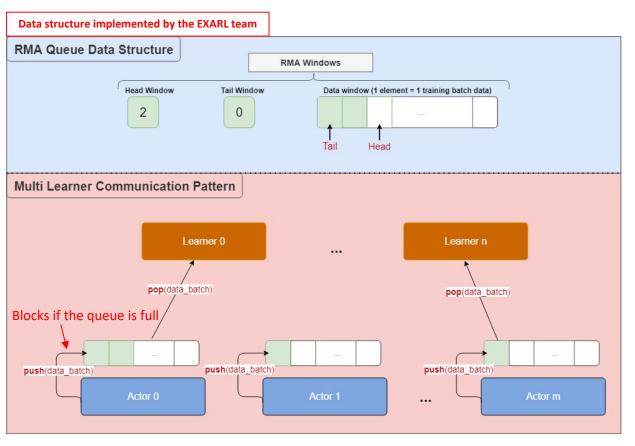
Random window selection

■Range based window selection



Range based window selection

Multi-learner RMA Queue Asynchronous workflow



Current approach

- Single learner.
- Communication pattern based on blocking MPI P2P routines.

RMA Queue approach

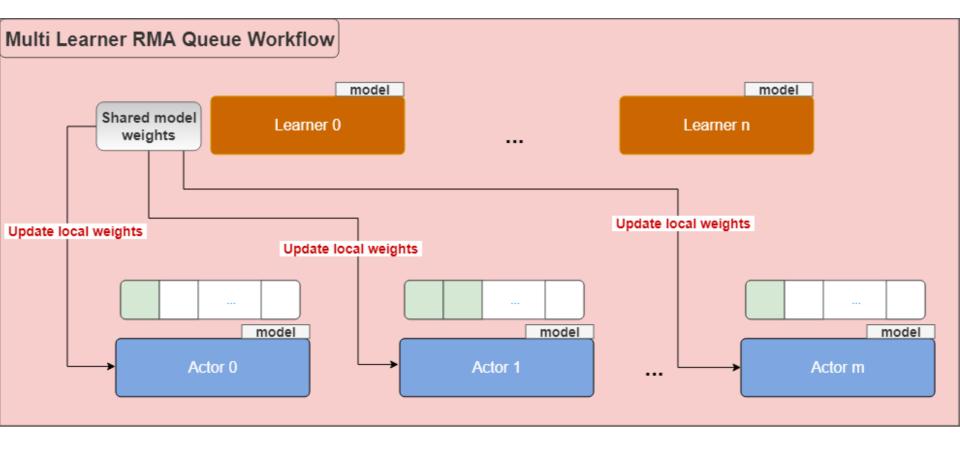
- Use the queue data structure from the current EXARL RMA workflow.
- Multi-learner communication pattern:
 - Actors interact with environment continuously and push batched training data to their local queue (blocks if the queue is full).
 - Each group of actors is assigned to a specific learner that pops training data randomly from its queue.

Advantages

- The actors and the learners are decoupled.
 - There is no active synchronization need.
- Multi-learner approach.

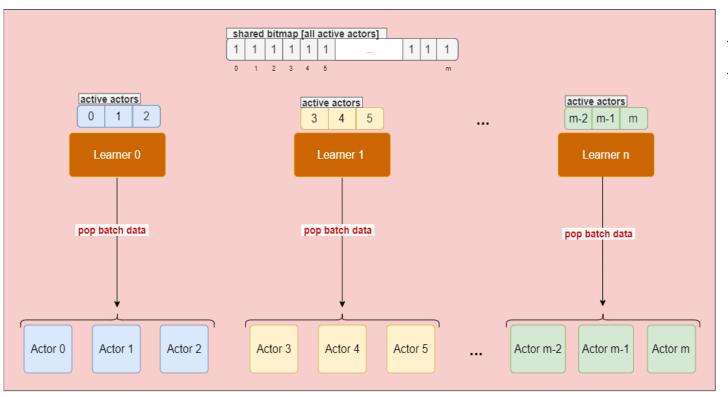


Multi-learner RMA Queue Asynchronous workflow





RMA Queue Asynchronous workflow – Implementation details

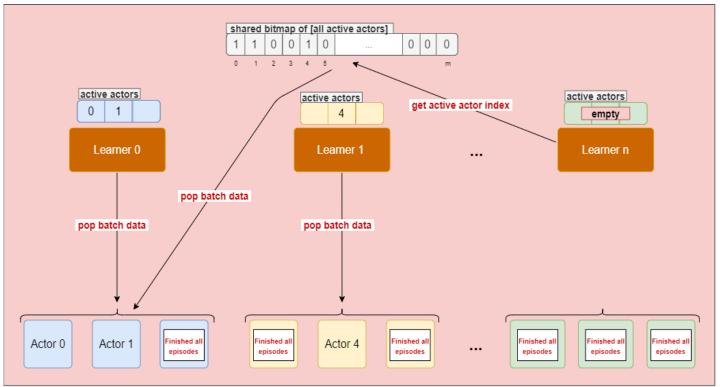


RMA Queue <u>approach</u>

 Each group of actors is assigned to a specific learner → allows to limit the number of simultaneous accesses to the same queue.



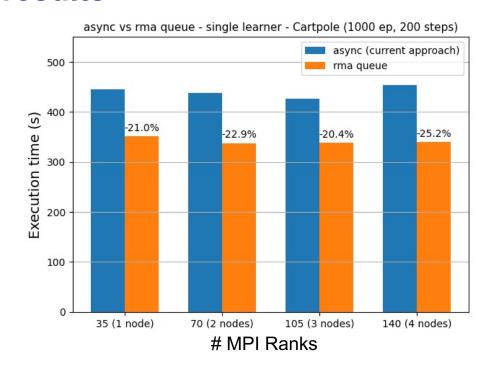
RMA Queue Asynchronous workflow – Implementation details



RMA Queue approach

- Learners that exhaust all 'active' actors assist other learners in fetching batch data.
- The "shared bitmap array" indicates which actors are active. This prevents getting data from an empty queue.

Multi-learner RMA Queue Asynchronous workflow – results



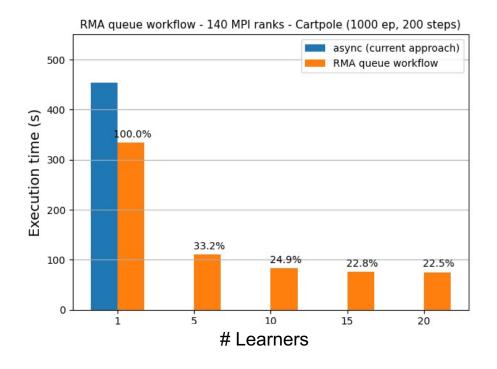
Single learner

- Achieved 25% performance improvement (on 4 nodes) compared to current asynchronous workflow.
- Limited Scalability: adding more actors didn't decrease the execution time → obvious need to increase concurrency through adding learners.

Limited Scalability → need to increase the number of learners



Multi-learner RMA Queue Asynchronous workflow – results

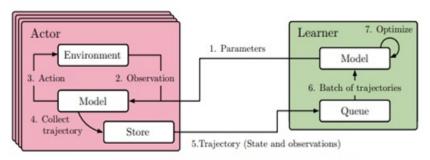


Multi-learner

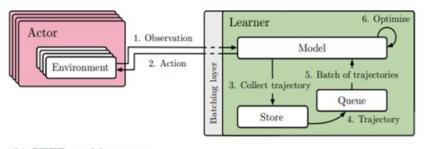
- Achieved 77% performance improvements (using 20 learners) compared to the single learner version.
- Good performance improvements for the same amount of hardware resources (140 processes).



SEED Architecture – moving the inference part to the learner



(a) IMPALA architecture (distributed version)



(b) SEED architecture SEED RL: http://arxiv.org/abs/1910.06591

SEED Advantages

- Using GPUs for neural network inference can result in execution time performance improvements for larger models
- As there is only one copy of the model, there is no issue of copies going out of sync
- Low bandwidth requirements relative to model parameters

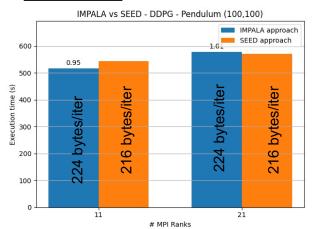
Current approach	SEED approach
Learner sends model weights	Learner sends the action to take
Actors send an entire training batch	Actors send a single observation

SEED Disadvantages

Can result in significant execution time increase for certain agents as the "generate_data()" function is called on the learner.

Example : DQN agent

SEED Results

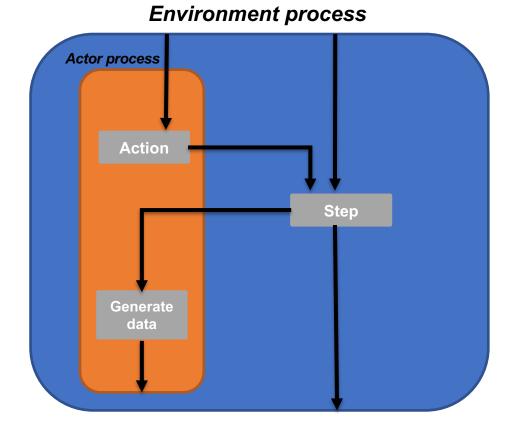




Accelerating DQN Data-Generation Pipeline

- Calculating Bellman optimality equation on each experience is expensive
 - 90% of computation time
- Current approach: Actor generates the training data
- Optimization: Offload data-generation on remaining environment processes
- Assumption: actor and environment does not execute simultaneously

Sampled experiences $q_*(s,a) = Eigg[R_{t+1} + \gamma \max_{a'} q_*ig(s',a'ig)igg]$ Batched training data

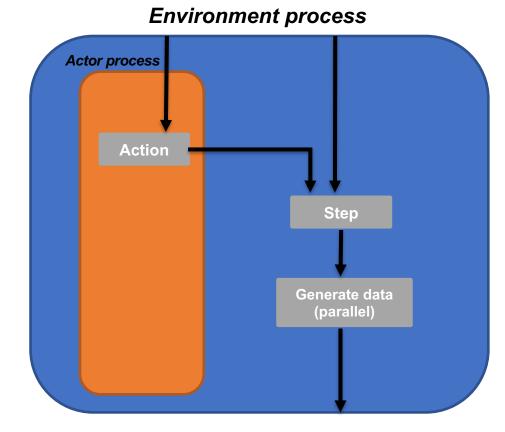




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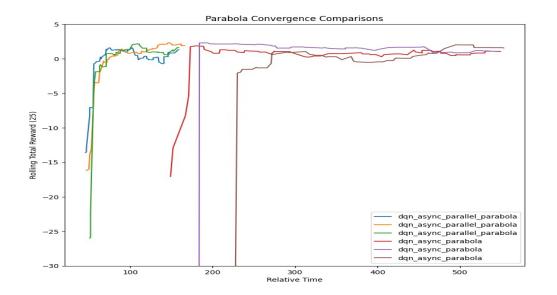


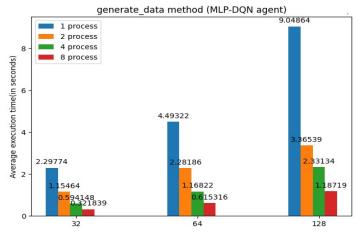


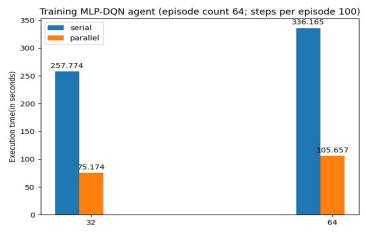
Accelerating DQN Data-Generation Pipeline

Results:

- Average speedup of 3.30x upon scaling the workload to 4 processes
- Faster convergence









Overview

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Improving Performance

- Scaling asynchronous workflow to multiple learners
- Improve scalability/execution time of multi-learner workflows
- Accelerate Deep Q-Network (DQN) data generation pipeline

Adding Functionalities

- New agents: Advantage Actor Critic (A2C/A3C), Twin Delayed Deep Deterministic Policy Gradient (TD3)
- V-trace algorithm
- Priority Experience Replay











(Asynchronous) Advantage Actor Critic (A2C/A3C)

Current Available Agent:

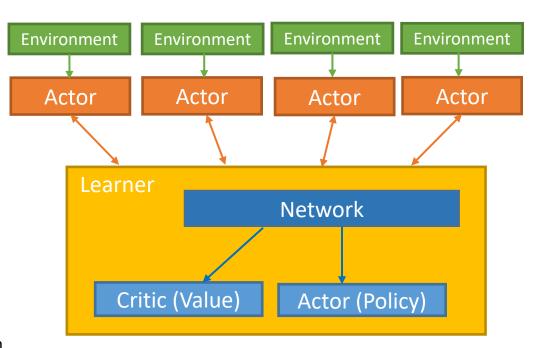
Deep Q-Network (DQN)

Limitations:

- DQN often takes a long time to train because it uses old data from replay buffer
- Training time is also long because of calculation of Bellman Equation

Update:

- A2C: synchronous workflow
- A3C: asynchronous workflow
- Faster to train & with more diverse data because each worker has their own environment for generating trajectories
- Current implementation is for <u>discrete action</u> <u>space environments</u>, but can be formulated for continuous ones, as well.





(Asynchronous) Advantage Actor Critic (A2C/A3C)

Current Available Agent:

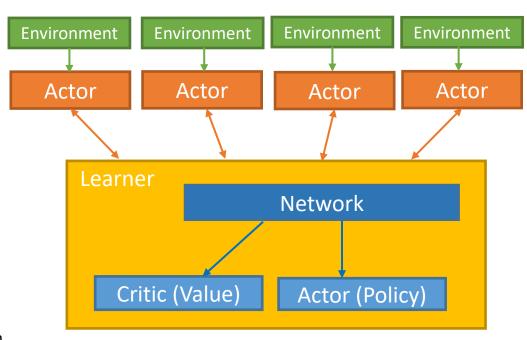
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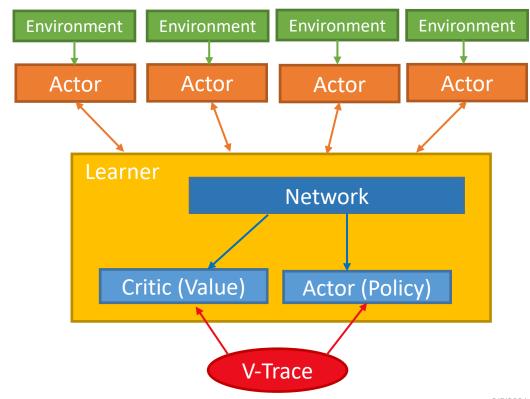


e.g. move left or right

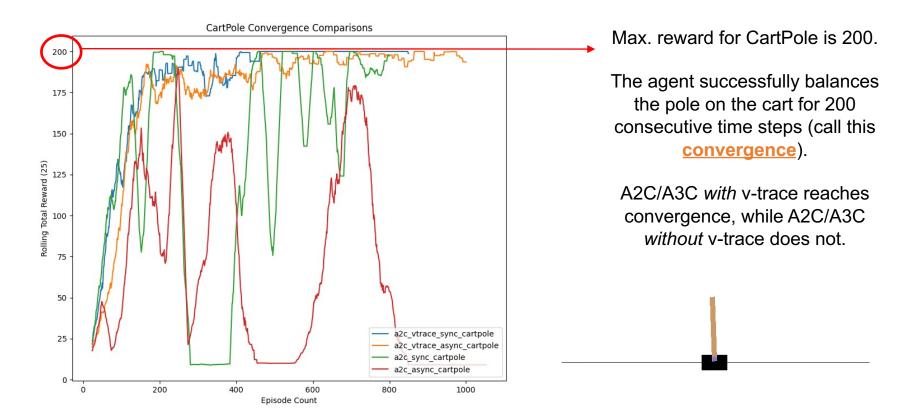


(Asynchronous) Advantage Actor Critic + V-Trace

- On-policy: the policy an actor acts with should be the same as the policy a learner learns with.
- In the EXARL framework, we can't always guarantee that they will have the same policy.
- To correct for that, we add an algorithm called "v-trace" to the loss functions.
- This correction assumes that the ratio between the two policies is always equal to one, therefore its addition forces this condition and we obtain the required on-policy behavior.

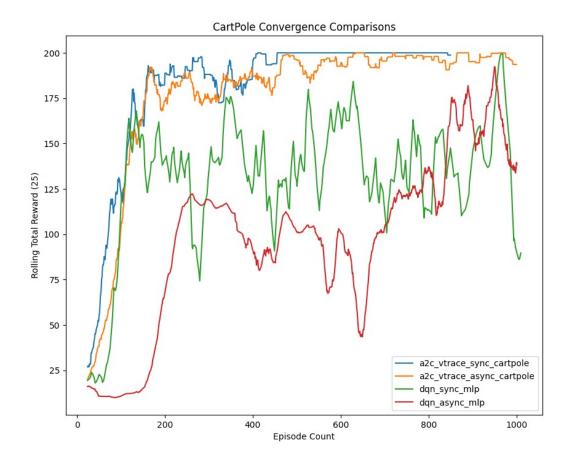






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A2C/A3C converge to expected value of 200 (CartPole environment), however DQN does not.

Results show DQN with Multi-Layer Perceptron (MLP) network, however results are similar for DQN with Long Short-Term Memory (LSTM) network.



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ExaBooster Environment

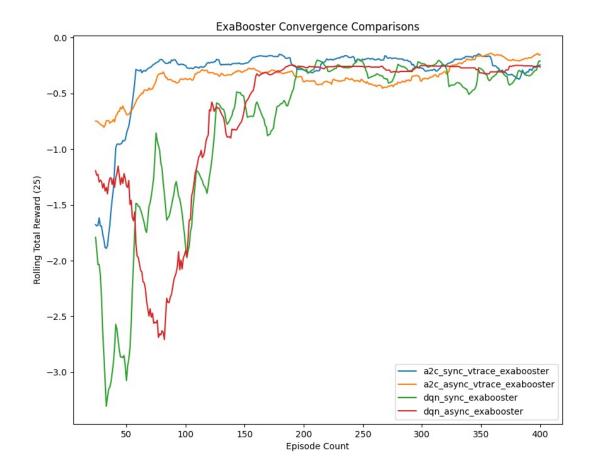
FNAL Accelerator Complex:



Courtesy: Christian Herwig

- Control problem for FNAL particle accelerator at FermiLab.
- Reinforcement learning is used to control particle beam quality (ie. reduce beam losses) in real time.
- Keeps the beam field from spreading (thus degrading the beam quality) by regulating the magnetic current of the booster.
- Original work developed by PNNL, FNAL, University of California San Diego, Columbia University





Convergence means: magnetic current is within some tolerance of an optimal value, which prevents too much spread in the beam field

A2C/A3C converges slightly faster than DQN (with LSTM network)



Added Agents

Current Available Agent for Continuous Action Space:

Deep Deterministic Policy Gradient (DDPG)

Limitations:

- It is frequently brittle to hyperparameters and other kinds of tuning
- The learned Q-function begins to overestimate Q-values which leads to policy breaking

Additions:

- Twin Delay Deep Deterministic policy gradient agent
- Prioritized Replay Buffer with Sumtree



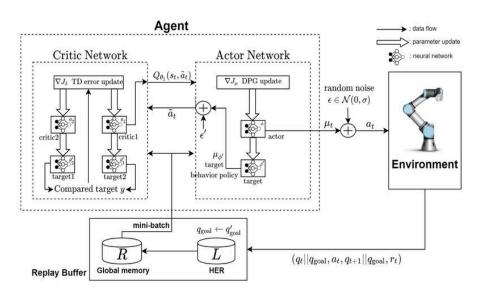
Twin Delay Deep Deterministic Policy Gradient (TD3)

Off-policy Agent: the policy an actor acts is independent on the policy a learner learns.

Twin Delay Deep Deterministic Policy Gradient Agent (TD3):

- Address the overestimate issue by using 3 tricks
 - Clicked Double Q-learning: Learns two Q-functions and uses the smaller of the two Q-values to form the targets in the Bellman error loss functions.
 - Delayed Policy agent: Updates the policy and target networks less frequently than the Q-function
 - Target policy smoothing: TD3 adds noise to the target action, to make it harder for the policy to exploit Q-function errors by smoothing out Q along the changes in action

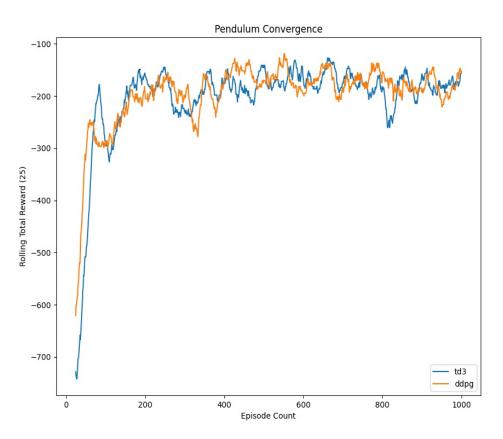
TD3 Architecture



https://www.researchgate.net/figure/Structure-of-TD3-Twin-Delayed-Deep-Deterministic-Policy-Gradient-with-RAMDP fig2 338605159



TD3 vs DDPG (Synchronous workflow)





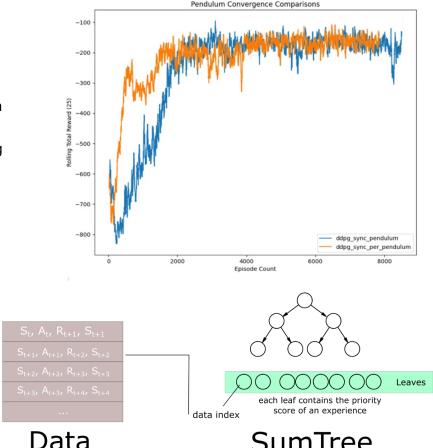
Effect of Replay Buffer

Uniform Sampling Replay Buffer

- Each transition sample in the minibatch is sampled uniformly from pool of stored experiences
- **Limitation**: When treating all samples the same, we are not using the fact that we can learn more from some experience

Prioritized Experience Replay Buffer

- Ranking of the experiences using the temporal-difference (TD) error (difference between the Q function and its target).
- Ranking of experiences by TD-error was done by storing the priority to experience mapping in a sum-tree.
- To avoid overfitting of our agent we update our policy network with important sampling weights.
- Sum-tree takes O(log n) for updating the tree and 0(1) to get the highest priority.



Data

SumTree



Summary/Conclusions: Performance Improvements

- We demonstrated improved scalability performance using efficient RMA communication patterns.
- Here we found that the total execution time decreased by 77% while using 20 learners and 120 actors on 4 nodes.
- We also created a multi-learner asynchronous workflow.
- Here we found there was a 43.4% increase in training throughput with 8 learners (actors = 8), training time reduced by 31% (actors = 16; learners = 8)
- We improved upon the existing framework by accelerating the data generation pipeline for the DQN agent for faster convergence.
- Here we found an average speedup of 3.30x when scaling the workload to 4 processes.



Summary/Conclusions: Adding Functionalities

- We expanded the capability of EXARL by including additional agents like (Asynchronized) Advantage Actor Critic (A2C/A3C) and Twin Delayed Deep Deterministic Policy Gradient (TD3)
- We also explored algorithmic improvements such as v-trace and Prioritized Experience Replay
- Here we found that A2C/A3C performed best with v-trace and outperformed Deep Q-Network (DQN) on both the CartPole game and the ExaBooster scientific environment.
- We also found that TD3 performed as good as the existing Deep Deterministic Policy Gradient (DDPG) agent
- We saw that adding Prioritized Experience Replay to DDPG accelerated convergence.



Acknowledgements



The Co-Design Summer School mentors:

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- Andrew Reisner
- Karen Tsai

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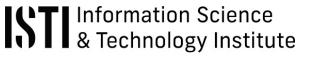
ECP, especially Christine Sweeney

Parallel Computing Summer Research Internship, especially Bob Robey

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Questions?

